

10558931.trn

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LOGINID:SSSPTA1626GMS

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 MAY 01 New CAS web site launched
NEWS 3 MAY 08 CA/CAPLUS Indian patent publication number format defined
NEWS 4 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 5 MAY 21 BIOSIS reloaded and enhanced with archival data
NEWS 6 MAY 21 TOXCENTER enhanced with BIOSIS reload
NEWS 7 MAY 21 CA/CAPLUS enhanced with additional kind codes for German patents
NEWS 8 MAY 22 CA/CAPLUS enhanced with IPC reclassification in Japanese patents
NEWS 9 JUN 27 CA/CAPLUS enhanced with pre-1967 CAS Registry Numbers
NEWS 10 JUN 29 STN Viewer now available
NEWS 11 JUN 29 STN Express, Version 8.2, now available
NEWS 12 JUL 02 LEMBASE coverage updated
NEWS 13 JUL 02 LMEDLINE coverage updated
NEWS 14 JUL 02 SCISEARCH enhanced with complete author names
NEWS 15 JUL 02 CHEMCATS accession numbers revised
NEWS 16 JUL 02 CA/CAPLUS enhanced with utility model patents from China
NEWS 17 JUL 16 CAPLUS enhanced with French and German abstracts
NEWS 18 JUL 18 CA/CAPLUS patent coverage enhanced
NEWS 19 JUL 26 USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 20 JUL 30 USGENE now available on STN
NEWS 21 AUG 06 CAS REGISTRY enhanced with new experimental property tags
NEWS 22 AUG 06 BEILSTEIN updated with new compounds
NEWS 23 AUG 06 FSTA enhanced with new thesaurus edition

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN. Columbus * * * * *

FILE 'HOME' ENTERED AT 14:18:22 ON 10 AUG 2007

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 14:18:31 ON 10 AUG 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 AUG 2007 HIGHEST RN 944380-35-2

DICTIONARY FILE UPDATES: 9 AUG 2007 HIGHEST RN 944380-35-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

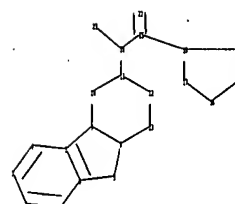
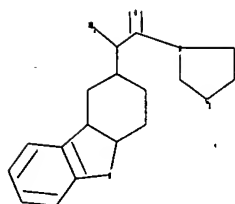
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

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chain nodes :

14 15 22 23

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 16 17 18 19 20

chain bonds :

11-14 14-15 14-23 15-18 15-22

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13
16-17 16-20 17-18 18-19 19-20

exact/norm bonds :

5-8 5-6 7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15 14-23 15-18
15-22 16-17 16-20 17-18 18-19 19-20

normalized bonds :

1-2 1-6 2-3 3-4 4-7 6-7

isolated ring systems :

containing 1 : 16 :

G1:S,CH2,CH,CF2,SO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 22:CLASS 23:CLASS

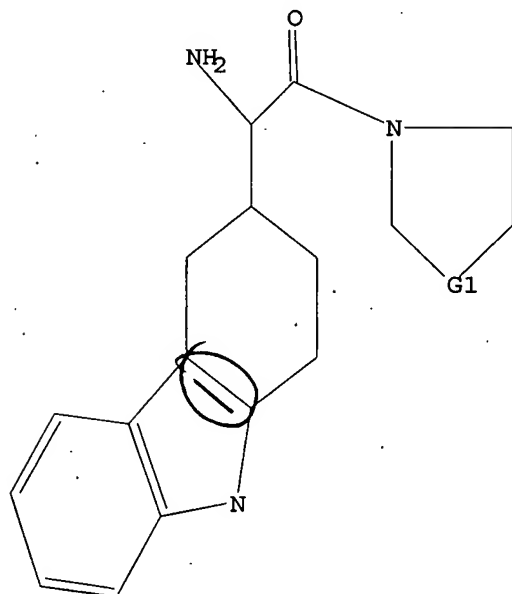
10558931.trn

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 14:18:46 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 14:18:53 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 52 TO ITERATE

100.0% PROCESSED 52 ITERATIONS

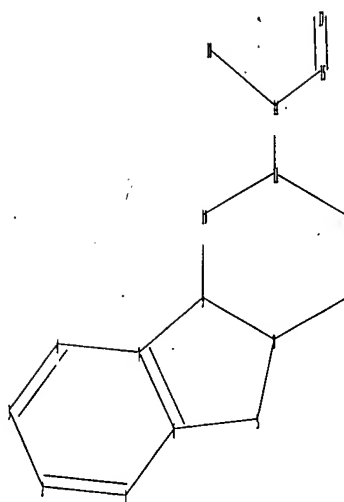
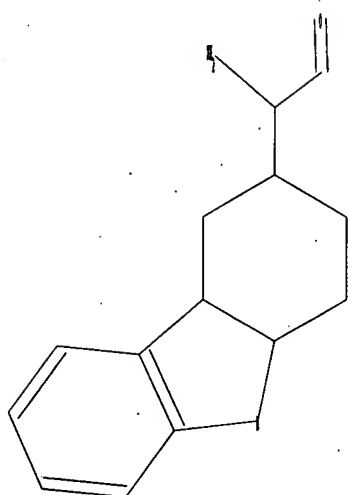
0 ANSWERS

SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=>

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```

chain nodes :
14 15 17 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
11-14 14-15 14-18 15-17
ring bonds :
1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13
exact/norm bonds :
5-8 5-6 14-18 15-17
exact bonds :
7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15
normalized bonds :
1-2 1-6 2-3 3-4 4-7 6-7
isolated ring systems :
containing 1 :
  
```

G1:S,CH2,CH,CF2,SO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 17:CLASS 18:CLASS

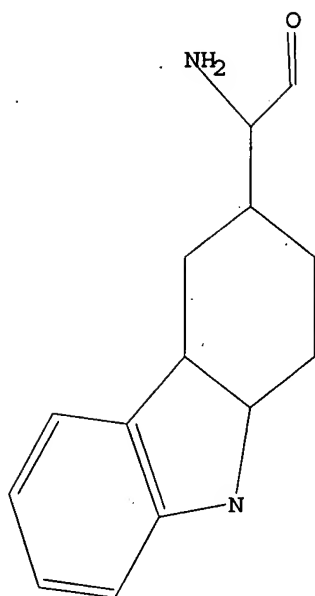
L4 STRUCTURE UPLOADED

=> d.14

L4 HAS NO ANSWERS

L4 STR

10558931.trn



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l4

SAMPLE SEARCH INITIATED 14:20:09 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 39 TO ITERATE

100.0% PROCESSED 39 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 406 TO 1154

PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s l4 sss full

FULL SEARCH INITIATED 14:20:15 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 740 TO ITERATE

100.0% PROCESSED 740 ITERATIONS

0 ANSWERS

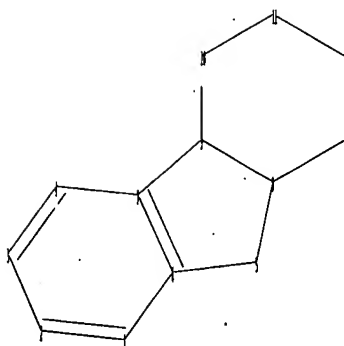
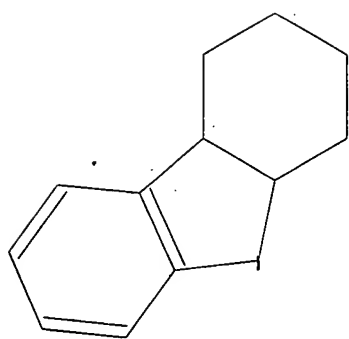
SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=>

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10558931.trn



ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13

exact/norm bonds :

5-8 5-6

exact bonds :

7-9 8-13 8-9 9-10 10-11 11-12 12-13

normalized bonds :

1-2 1-6 2-3 3-4 4-7 6-7

isolated ring systems :

containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom

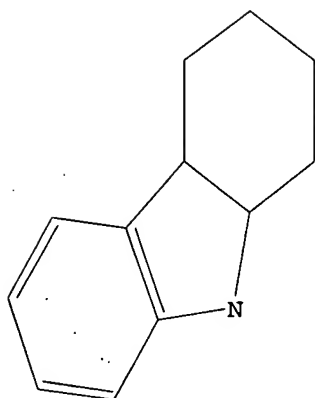
L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR

10558931.trn



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s 17

SAMPLE SEARCH INITIATED 14:21:33 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2011 TO ITERATE

99.5% PROCESSED 2000 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 37530 TO 42910

PROJECTED ANSWERS: 740 TO 1672

L8 50 SEA SSS SAM L7

=> s 17 sss full

FULL SEARCH INITIATED 14:21:40 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 38933 TO ITERATE

100.0% PROCESSED 38933 ITERATIONS

1220 ANSWERS

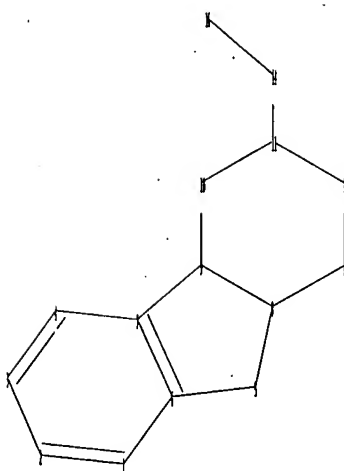
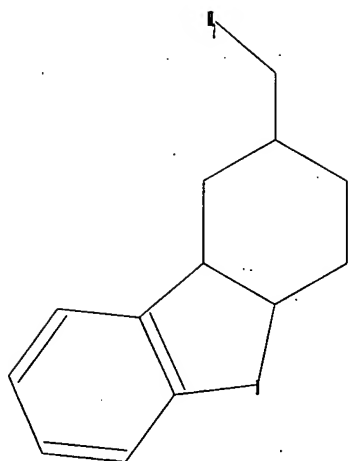
SEARCH TIME: 00.00.01

L9 1220 SEA SSS FUL L7

=>

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10558931.trn



chain nodes :

14 16

ring nodes :.

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

11-14 14-16

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13

exact/norm bonds :

5-8 5-6 14-16

exact bonds :

7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13

normalized bonds :

1-2 1-6 2-3 3-4 4-7 6-7

isolated ring systems :

containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:CLASS 16:CLASS

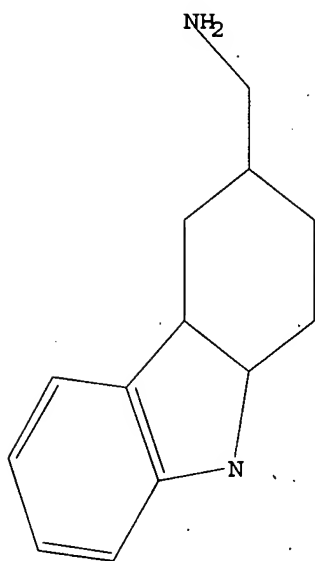
L10 STRUCTURE UPLOADED

=> d l10

L10 HAS NO ANSWERS

L10 STR

10558931.trn



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l10

SAMPLE SEARCH INITIATED 14:22:55 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 216 TO ITERATE

100.0% PROCESSED 216 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3439 TO 5201
PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L10

=> s l10 sss full

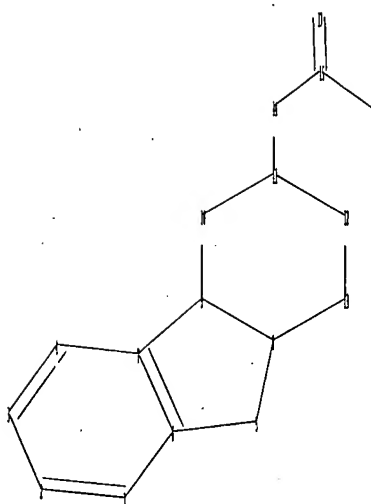
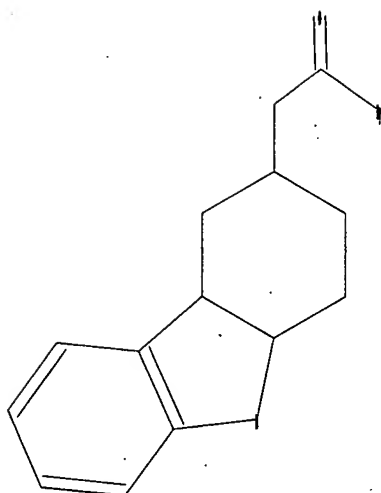
FULL SEARCH INITIATED 14:23:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3888 TO ITERATE

100.0% PROCESSED 3888 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L12 0 SEA SSS FUL L10

=>

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```

chain nodes :
14 15 17 19
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
11-14 14-15 15-17 15-19
ring bonds :
1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13
exact/norm bonds :
5-8 5-6 15-17 15-19
exact bonds :
7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15
normalized bonds :
1-2 1-6 2-3 3-4 4-7 6-7
isolated ring systems :
containing 1 :

```

G1:S,CH2,CH,CF2,SO2

Match level :

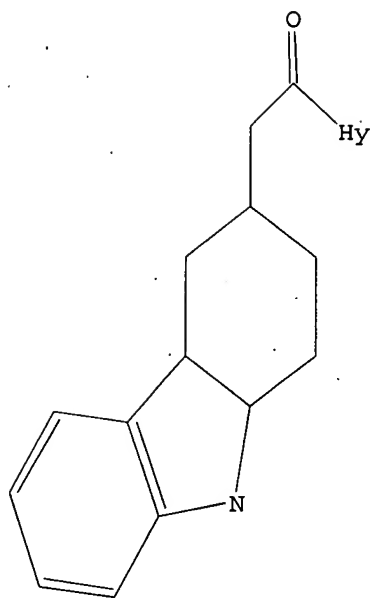
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 17:CLASS 19:CLASS

L13 STRUCTURE UPLOADED

=> d l13

L13 HAS NO ANSWERS

L13 STR



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l13

SAMPLE SEARCH INITIATED 14:24:43 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 244 TO ITERATE

100.0% PROCESSED 244 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 3943 TO 5817

PROJECTED ANSWERS: 0 TO 0

L14 0 SEA SSS SAM L13

=> s l13 sss full

FULL SEARCH INITIATED 14:24:50 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 4979 TO ITERATE

100.0% PROCESSED 4979 ITERATIONS

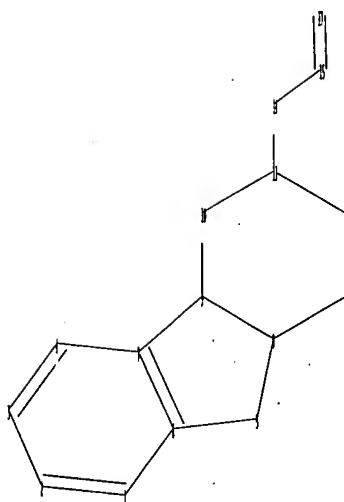
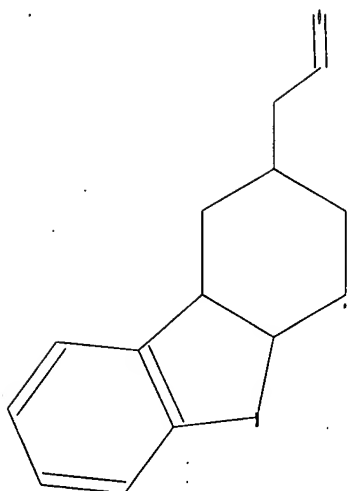
0 ANSWERS

SEARCH TIME: 00.00.01

L15 0 SEA SSS FUL L13

=>

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```

chain nodes :
14 15 17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
11-14 14-15 15-17
ring bonds :
1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13
exact/norm bonds :
5-8 5-6 15-17
exact bonds :
7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15
normalized bonds :
1-2 1-6 2-3 3-4 4-7 6-7
isolated ring systems :
containing 1 :
  
```

G1:S,CH2,CH,CF2,SO2

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 17:CLASS
  
```

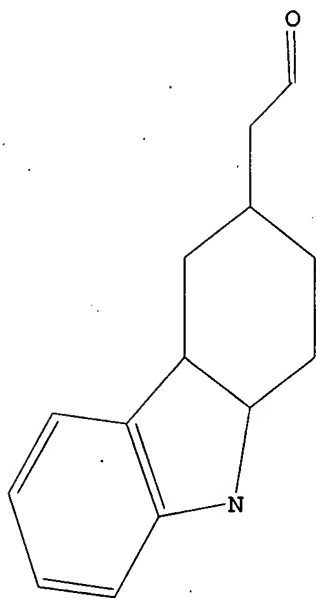
L16 STRUCTURE UPLOADED

=> d l16

L16 HAS NO ANSWERS

L16 STR

10558931.trn



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l16

SAMPLE SEARCH INITIATED 14:27:21 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 244 TO ITERATE

100.0% PROCESSED 244 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 3943 TO 5817

PROJECTED ANSWERS: 0 TO 0

L17 0 SEA SSS SAM L16

=> s l16 sss full

FULL SEARCH INITIATED 14:27:29 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 4979 TO ITERATE

100.0% PROCESSED 4979 ITERATIONS

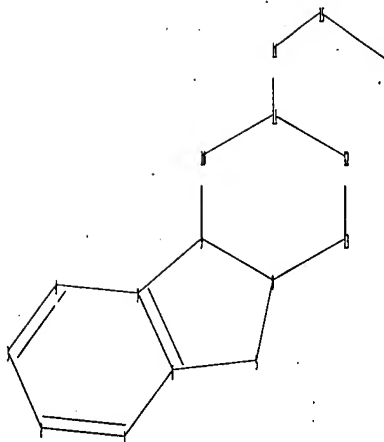
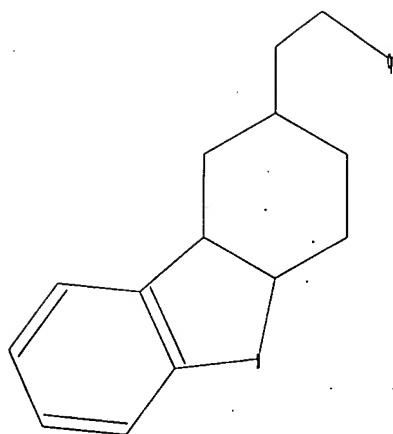
0 ANSWERS

SEARCH TIME: 00.00.01

L18 0 SEA SSS FUL L16

=>

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```

chain nodes :
14 15 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
11-14 14-15 15-18
ring bonds :
1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13
exact/norm bonds :
5-8 5-6 15-18
exact bonds :
7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15
normalized bonds :
1-2 1-6 2-3 3-4 4-7 6-7
isolated ring systems :
containing 1 :

```

G1:S,CH2,CH,CF2,SO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 18:CLASS

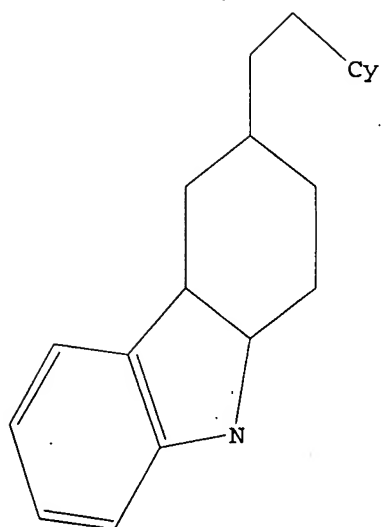
L19 STRUCTURE UPLOADED

=> d l19

L19 HAS NO ANSWERS

L19 STR

10558931.trn



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l19

SAMPLE SEARCH INITIATED 14:30:04 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 954 TO ITERATE

100.0% PROCESSED 954 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 17227 TO 20933

PROJECTED ANSWERS: 0 TO 0

L20 0 SEA SSS SAM L19

=> s l19 sss full

FULL SEARCH INITIATED 14:30:11 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 17864 TO ITERATE

100.0% PROCESSED 17864 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L21 0 SEA SSS FUL L19

=> d his

(FILE 'HOME' ENTERED AT 14:18:22 ON 10 AUG 2007)

FILE 'REGISTRY' ENTERED AT 14:18:31 ON 10 AUG 2007

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 SSS FULL

L4 STRUCTURE UPLOADED

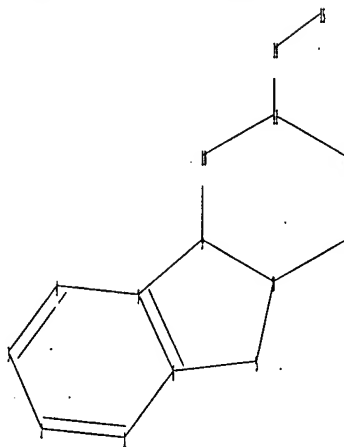
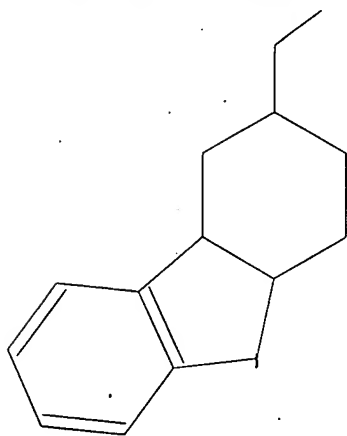
L5 0 S L4

10558931.trn

L6 0 S L4 SSS FULL
L7 STRUCTURE UPLOADED
L8 50 S L7
L9 1220 S L7 SSS FULL
L10 STRUCTURE UPLOADED
L11 0 S L10
L12 0 S L10 SSS FULL
L13 STRUCTURE UPLOADED
L14 0 S L13
L15 0 S L13 SSS FULL
L16 STRUCTURE UPLOADED
L17 0 S L16
L18 0 S L16 SSS FULL
L19 STRUCTURE UPLOADED
L20 0 S L19
L21 0 S L19 SSS FULL

=>

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chain nodes :

14 15

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

11-14 14-15

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13

exact/norm bonds :

5-8 5-6

exact bonds :

7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15

normalized bonds :

1-2 1-6 2-3 3-4 4-7 6-7

isolated ring systems :

containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS

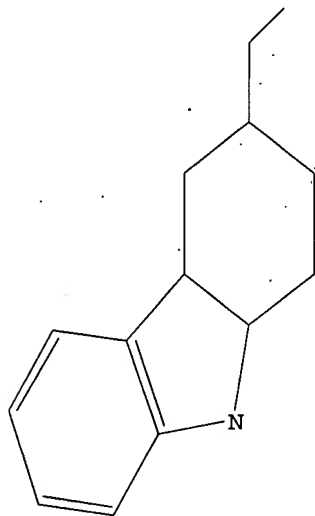
10558931.trn

L22 STRUCTURE UPLOADED

=> d l22

L22 HAS NO ANSWERS

L22 STR



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l22

SAMPLE SEARCH INITIATED 14:32:19 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1082 TO ITERATE

100.0% PROCESSED 1082 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 19667 TO 23613

PROJECTED ANSWERS: 2 TO 124

L23 2 SEA SSS SAM L22

=> s l22 sss full

FULL SEARCH INITIATED 14:32:30 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 20417 TO ITERATE

100.0% PROCESSED 20417 ITERATIONS

36 ANSWERS

SEARCH TIME: 00.00.01

L24 36 SEA SSS FUL L22

=> d his

10558931.trn

(FILE 'HOME' ENTERED AT 14:18:22 ON 10 AUG 2007)

FILE 'REGISTRY' ENTERED AT 14:18:31 ON 10 AUG 2007

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 0 S L1 SSS FULL
L4 STRUCTURE UPLOADED
L5 0 S L4
L6 0 S L4 SSS FULL
L7 STRUCTURE UPLOADED
L8 50 S L7
L9 1220 S L7 SSS FULL
L10 STRUCTURE UPLOADED
L11 0 S L10
L12 0 S L10 SSS FULL
L13 STRUCTURE UPLOADED
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L15 0 S L13 SSS FULL
L16 STRUCTURE UPLOADED
L17 0 S L16
L18 0 S L16 SSS FULL
L19 STRUCTURE UPLOADED
L20 0 S L19
L21 0 S L19 SSS FULL
L22 STRUCTURE UPLOADED
L23 2 S L22
L24 36 S L22 SSS FULL

=> FIL HCAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

1384.00

1384.21

FILE 'HCAPLUS' ENTERED AT 14:33:02 ON 10 AUG 2007

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FILE COVERS 1907 - 10 Aug 2007 VOL 147 ISS 8

FILE LAST UPDATED: 9 Aug 2007 (20070809/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l24

L25 15 L24

10558931.trn

=> s 19

L26 472 L9

=> s 125 and py<=2003

23927587 PY<=2003

L27 14 L25 AND PY<=2003

=> s 126 and p/dt

5818845 P/DT

L28 127 L26 AND P/DT

=> s 128 and us/pc

1705037 US/PC

L29 57 L28 AND US/PC

=> s 129 and py<=2003

23927587 PY<=2003

L30 51 L29 AND PY<=2003

=> s 130 and dipeptidyl

4690 DIPEPTIDYL

L31 0 L30 AND DIPEPTIDYL

=> s 130 and thu

159 THU

2428717 THUS

2428858 THU

(THU OR THUS)

L32 28 L30 AND THU

=> s 132 and diabetes

128376 DIABETES

L33 0 L32 AND DIABETES

=> s 132 and disease

978988 DISEASE

264275 DISEASES

1096696 DISEASE

(DISEASE OR DISEASES)

L34 4 L32 AND DISEASE

=> d his

(FILE 'HOME' ENTERED AT 14:18:22 ON 10 AUG 2007)

FILE 'REGISTRY' ENTERED AT 14:18:31 ON 10 AUG 2007

L1 STRUCTURE UPLOADED
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L14 0 S L13

10558931.trn

L15 0 S L13 SSS FULL
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L20 0 S L19
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L22 STRUCTURE UPLOADED
L23 2 S L22
L24 36 S L22 SSS FULL

FILE 'HCAPLUS' ENTERED AT 14:33:02 ON 10 AUG 2007

L25 15 S L24
L26 472 S L9
L27 14 S L25 AND PY<=2003
L28 127 S L26 AND P/DT
L29 57 S L28 AND US/PC
L30 51 S L29 AND PY<=2003
L31 0 S L30 AND DIPEPTIDYL
L32 28 S L30 AND THU
L33 0 S L32 AND DIABETES
L34 4 S L32 AND DISEASE

=> d l25 ibib abs hitstr tot

L25 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:656254 HCAPLUS

DOCUMENT NUMBER: 145:125169

TITLE: Rigid amines for use in manufacture of conjugated polymer useful as emitters, charge transporters or host materials in opto-electrical devices

INVENTOR(S): Heidenhain, Sophie; Leadbeater, Mark; Steudel, Annette; Hicks, Daniel

PATENT ASSIGNEE(S): Cambridge Display Technology Limited, UK; CDT Oxford Limited

SOURCE: PCT Int. Appl., 49 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006070185	A1	20060706	WO 2005-GB5058	20051223
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.:

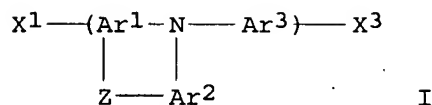
GB 2004-28443

A 20041229

GB 2005-2254

A 20050203

GI

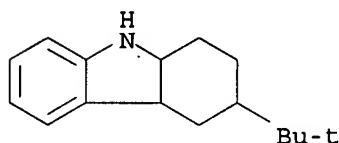


AB The monomer has a structure as shown in I where: Ar1, Ar2 and Ar3 are independently selected from optionally substituted aryl or heteroaryl, X1 and X3 both independently comprise a leaving group capable of participating in polymerization and Z represents a direct bond or an optionally substituted bridging atom.

IT 6731-89-1P
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
 (manufacture of rigid amines as monomers for conjugated polymer useful for emitters, charge transporters or host materials in opto-elec. devices)

RN 6731-89-1 HCAPLUS

CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:363554 HCAPLUS

DOCUMENT NUMBER: 131:115858

TITLE: Alkylation of ketone and ester lithium enolates with nitroethylene

AUTHOR(S): Flintoft, Rebecca J.; Buzby, Jennifer C.; Tucker, John A.

CORPORATE SOURCE: Medicinal Chemistry Research, Pharmacia and Upjohn, Kalamazoo, MI, 49001, USA

SOURCE: Tetrahedron Letters (1999), 40(24), 4485-4488
 CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 131:115858

AB We describe the first systematic study of the scope and limitations of the conjugate addition of ketone and ester enolates to nitroethylene. Synthetically useful yields are obtained for ketone and ester enolates of a variety of structural types.

IT 232923-95-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkylation of ketone enolates or ester enolates with nitroethylene)

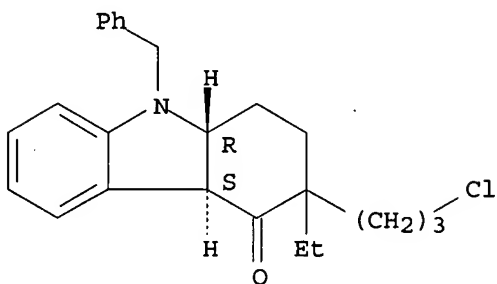
RN 232923-95-4 HCAPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-

10558931.trn

(phenylmethyl)-, (4aR,9aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 232924-06-0P

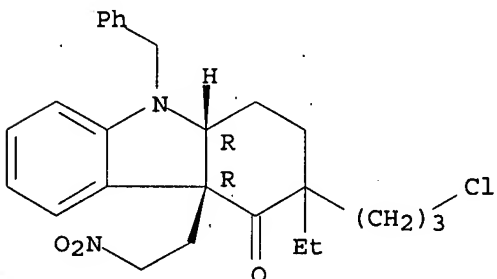
RL: SPN (Synthetic preparation); PREP (Preparation)

(alkylation of ketone enolates or ester enolates with nitroethylene)

RN 232924-06-0 HCAPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (4aR,9aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:631122 HCAPLUS

DOCUMENT NUMBER: 121:231122

TITLE: Unexpected results in the reduction of tetracyclic enamides. Structure, stereochemistry and conformation of a 20 β -hydroperoxyimine

AUTHOR(S): Dugat, Denise; Dauphin, Gerard; Gramain, Jean-Claude
CORPORATE SOURCE: Universite Blaise Pascal de Clermont-Ferrand, Aubiere, 63177, Fr.

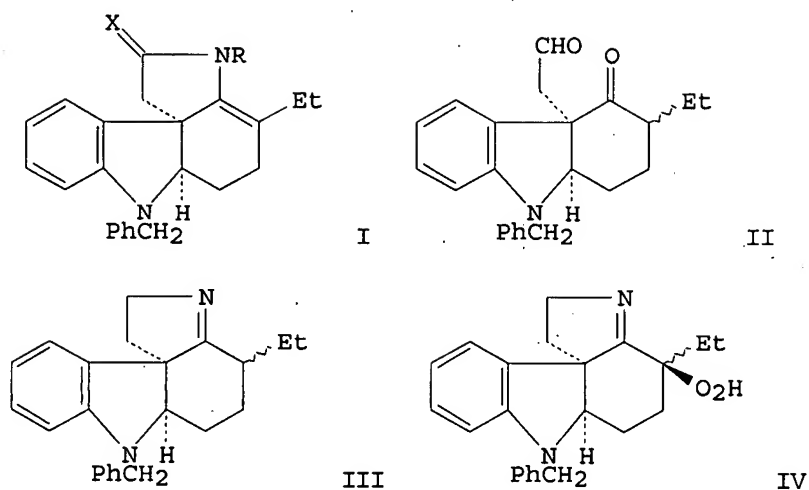
SOURCE: Heterocycles (1994), 38(8), 1909-18

CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Reduction of Nb-allyl-20-ethyltetracyclic enamide I (X = O, R = allyl) with lithium aluminum hydride afforded the expected enamine I (X = H₂, R = allyl) and 4a-oxoethylhexahydrocarbazolones II. Reduction of Nb-unsubstituted enamide I (X = O, R = H), under the same conditions, gave imine III, enamine I (X = H₂, R = H) and a 20β-hydroperoxytetracyclic imine IV resulting from peroxydation. The C-20 stereochem. of IV was established by means of 2D 1H NMR and NOE difference spectroscopy.

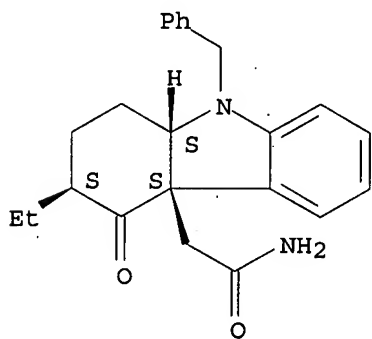
IT 158148-36-8P 158148-37-9P 158148-38-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and intramol. cyclization of)

RN 158148-36-8 HCAPLUS

CN 4aH-Carbazole-4a-acetamide, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3α,4α,9α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

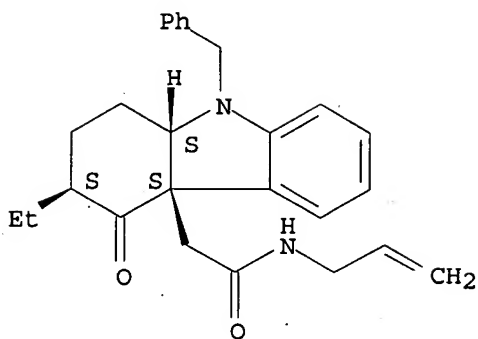


RN 158148-37-9 HCAPLUS

CN 4aH-Carbazole-4a-acetamide, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-N-2-propenyl-, (3α,4α,9α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

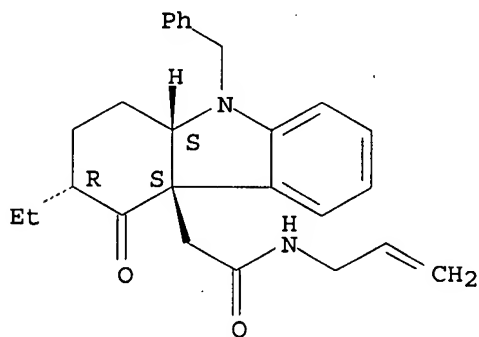
10558931.trn



RN 158148-38-0 HCAPLUS

CN 4aH-Carbazole-4a-acetamide, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-N-2-propenyl-, (3 α ,4 $\alpha\beta$,9 $\alpha\beta$)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



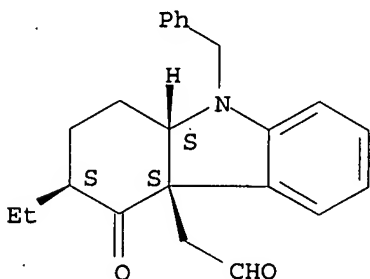
IT 158148-44-8P 158148-45-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 158148-44-8 HCAPLUS

CN 4aH-Carbazole-4a-acetaldehyde, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3 α ,4 $\alpha\alpha$,9 $\alpha\alpha$)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

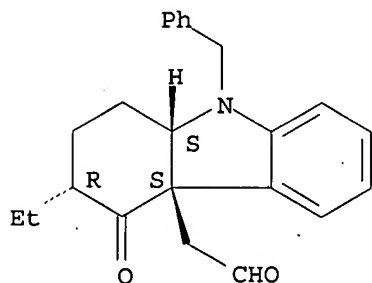


RN 158148-45-9 HCAPLUS

CN 4aH-Carbazole-4a-acetaldehyde, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3 α ,4 $\alpha\beta$,9 $\alpha\beta$)- (9CI) (CA INDEX NAME)

10558931.trn

Relative stereochemistry.



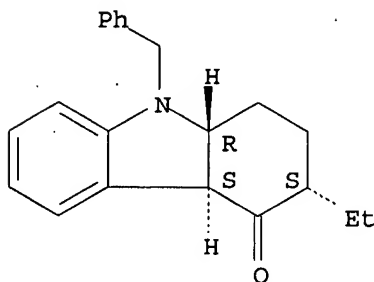
IT 129574-42-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with iodoacetamide)

RN 129574-42-1 HCAPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-,
(3 α ,4 α ,9a β) - (9CI) (CA INDEX NAME)

Relative stereochemistry.



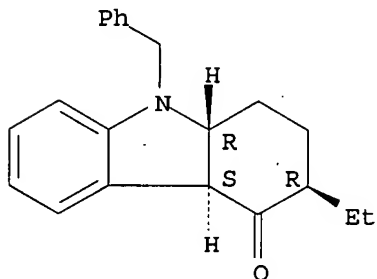
IT 129574-41-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with iodoacetamides)

RN 129574-41-0 HCAPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-,
(3 α ,4 α ,9a α) - (9CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:134890 HCAPLUS

10558931.trn

DOCUMENT NUMBER: 120:134890
TITLE: Stereocontrolled formation of octahydro-1H-pyrrolo[2,3-d]carbazoles by reductive cyclization: total synthesis of (+)-N-benzylaspidospermidine
AUTHOR(S): Benchekroun-Mounir, Nora; Dugat, Denise; Gramain, Jean Claude; Husson, Henri Philippe
CORPORATE SOURCE: URA, Univ. Blaise Pascal Clermont-Ferrand, Aubiere, 63177, Fr.
SOURCE: Journal of Organic Chemistry (1993), 58(23), 6457-65
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:134890
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The synthesis of a series of 20-substituted octahydro-1H-pyrrolo[2,3-d]carbazoles, intermediates in the synthesis of Aspidosperma alkaloids, is described. Nonoxidative photocyclization of aryl enaminone I led to hexahydrocarbazol-4-ones II. Alkylation of the anions derived from II with KH and iodoacetonitrile gave rise to an undesirable intramol. cyclization while reaction with LDA and nitroethylene as Michael acceptor afforded the trisubstituted hexahydrocarbazolones III (R = CH₂CH₂CH₂Cl). Reductive cyclization (H₂, PtO₂) of cyano model compds. provided octahydro-1H-pyrrolo[2,3-d]carbazoles whose stereochem. depended on hindrance of the α and β face of the mol. In contrast, reduction (HCOONH₄, Pd/C, and then Na/EtOH) of nitro model compds. III (R = H) via nitrones led essentially to the more stable isomers IV with the natural stereochem. at C-21. Reduction (HCOONH₄, Pd/C) of nitro compds. III (R = CH₂CH₂CH₂Cl), which possess the elements for the future construction of the D and E rings, induced a tandem cyclization and afforded the pentacyclic iminium which was converted by catalytic hydrogenation into (+)-N-benzylaspidospermidine (V). This compound was thus synthesized in seven steps from N-benzylaniline and cyclohexane-1,3-dione.

IT 129574-41-0 129574-43-2

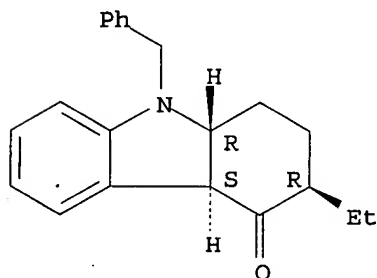
RL: PROC (Process)

(addition of, with nitroethylene)

RN 129574-41-0 HCAPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3 α ,4 α β ,9 α)- (9CI) (CA INDEX NAME)

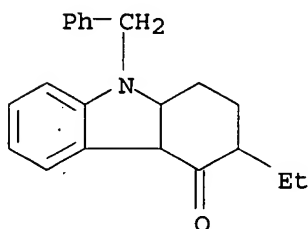
Relative stereochemistry.



RN 129574-43-2 HCAPLUS

10558931.trn

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-,
(3 α ,4 α ,9 α)- (9CI) (CA INDEX NAME)



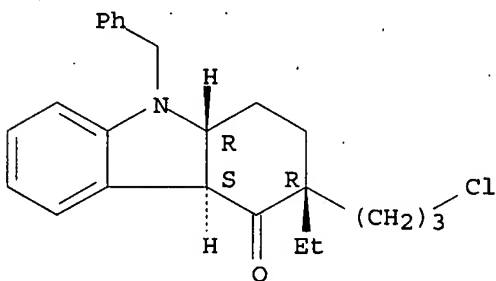
IT 143466-44-8P 143466-49-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and addition of, with nitroethylene)

RN 143466-44-8 HCAPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-
(phenylmethyl)-, (3 α ,4 α ,9 α)- (9CI) (CA INDEX NAME)

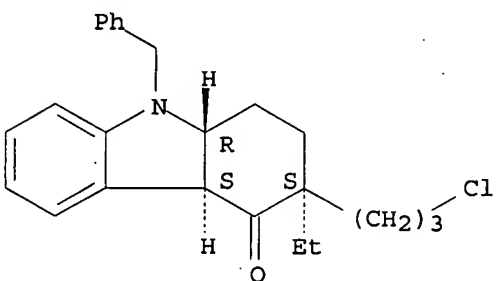
Relative stereochemistry.



RN 143466-49-3 HCAPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-
(phenylmethyl)-, (3 α ,4 α ,9 α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 152710-80-0P 152710-81-1P 152710-89-9P

152710-90-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reduction of)

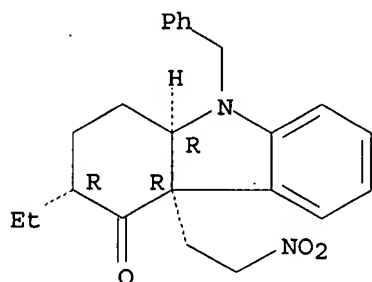
RN 152710-80-0 HCAPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-

10558931.trn

(phenylmethyl)-, (3 α ,4 α ,9 α)- (9CI) (CA INDEX NAME)

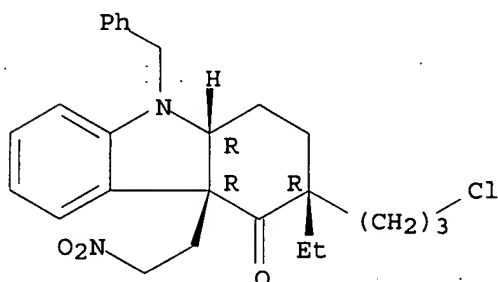
Relative stereochemistry.



RN 152710-81-1 HCAPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3 α ,4 α β ,9 α β)- (9CI) (CA INDEX NAME)

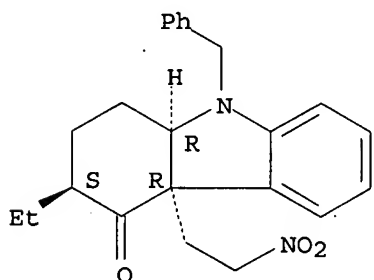
Relative stereochemistry.



RN 152710-89-9 HCAPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3 α ,4 α β ,9 α β)- (9CI) (CA INDEX NAME)

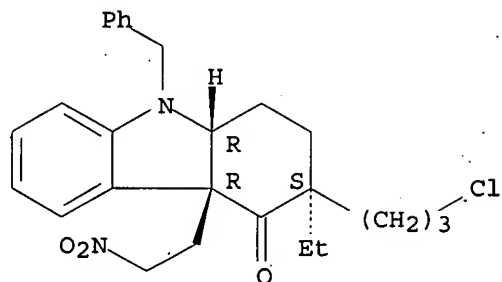
Relative stereochemistry.



RN 152710-90-2 HCAPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3 α ,4 α ,9 α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 152710-78-6P

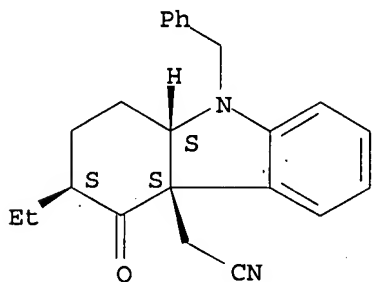
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reductive intramol. cyclization of)

RN 152710-78-6 HCAPLUS

CN 4aH-Carbazole-4a-acetonitrile, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3 α ,4 α ,9 α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



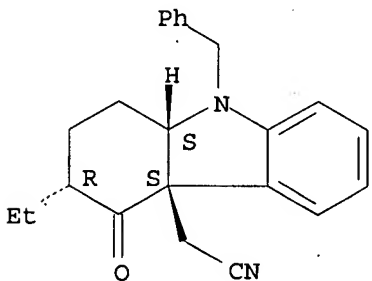
IT 152710-88-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 152710-88-8 HCAPLUS

CN 4aH-Carbazole-4a-acetonitrile, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3 α ,4 α ,9 α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



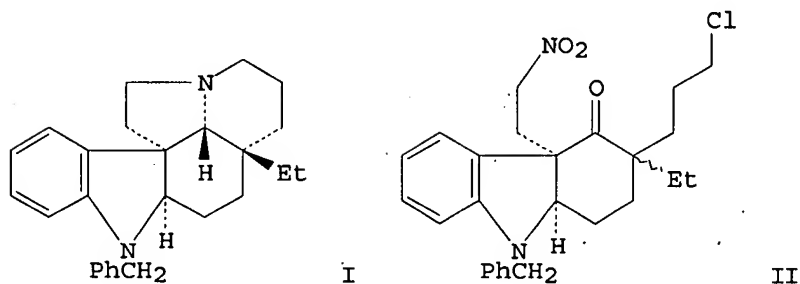
L25 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:571783 HCAPLUS

DOCUMENT NUMBER: 117:171783

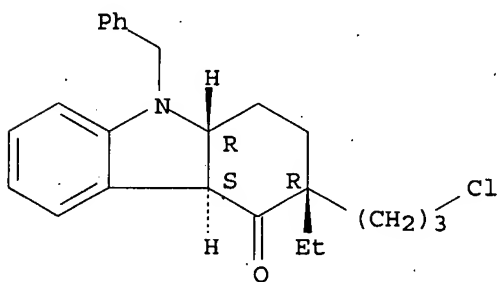
TITLE: A short synthesis of (\pm)-N-benzyl aspidospermidine

AUTHOR(S): Benchekroun-Mounir, Nora; Dugat, Denise; Gramain, Jean Claude
 CORPORATE SOURCE: Univ. Blaise Pascal de Clermont-Ferrand, Aubiere, 63177, Fr.
 SOURCE: Tetrahedron Letters (1992), 33(28), 4001-4
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 117:171783
 GI



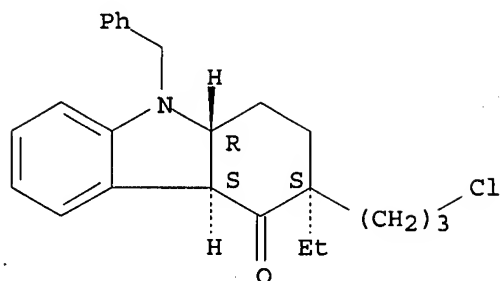
AB (+)-N-Benzyl aspidospermidine (I) is synthesized in seven steps via the trisubstituted hexahydrocarbazolone II; reductive cyclization of this intermediate which is obtained by photocyclization and Michael reaction with nitroethylene, creates simultaneously both E and D rings of the pentacyclic system.
 IT 143466-44-8P 143466-49-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and alkylation of, with nitroethylene)
 RN 143466-44-8 HCAPLUS
 CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3 α ,4 α ,9 α)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 143466-49-3 HCAPLUS
 CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3 α ,4 α ,9 α)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



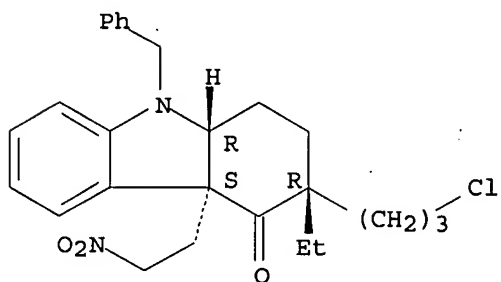
IT 143466-45-9P 143466-48-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reductive cyclization of)

RN 143466-45-9 HCAPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3 α ,4 α ,9 $\alpha\beta$)-(9CI) (CA INDEX NAME)

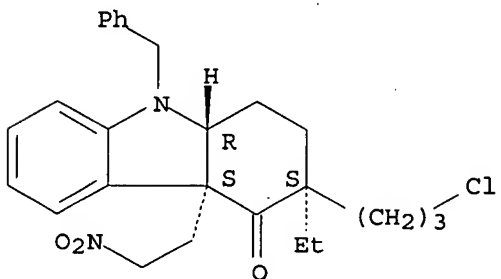
Relative stereochemistry.



RN 143466-48-2 HCAPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3 α ,4 $\alpha\beta$,9 $\alpha\alpha$)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:552186 HCAPLUS

DOCUMENT NUMBER: 113:152186

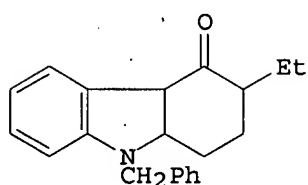
TITLE: Structure, stereochemistry, and conformation of

AUTHOR(S):
CORPORATE SOURCE:

SOURCE:

DOCUMENT TYPE:
LANGUAGE:
OTHER SOURCE(S):
GI

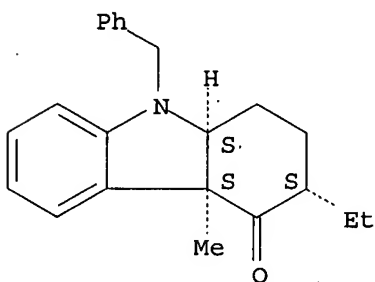
diastereoisomeric cis- and trans-3-ethyl-1,2,3,4,4a,9a-hexahydrocarbazol-4-ones by means of ^{13}C and two-dimensional proton NMR spectroscopy. An example of diastereoselection in a photocyclization reaction Dugat, Denise; Gramain, Jean Claude; Dauphin, Gerard Unite Rech., Univ. Blaise Pascal Clermont-Ferrand, Aubiere, 63177, Fr. Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1990), (4), 605-11 CODEN: JCPKBH; ISSN: 0300-9580 Journal English CASREACT 113:152186



I

- AB Diastereoisomers of 3-ethylhexahydrocarbazol-4-one (I) are stereospecifically obtained in a 4a,9a-trans-configuration by a photocyclization reaction in which appreciable diastereoselection (40%) due to the Et chain is observed. They are quant. converted to cis compds. by treatment with acid or by angular alkylation via a benzylic carbanion. Complete anal. of the ^1H (1D, 2D) NMR spectra allows the conformation of the C ring in each compound to be established. Moreover, the collected ^1H and ^{13}C NMR data constitute refs. for further identification of the cis and trans series and further determination of the position of the 3-Et chain. Equilibrium studies between the different isomers show the higher stability of the cis derivs. which possess the configuration of the natural products of the *Aspidosperma* indole alkaloids.
- IT 129574-45-4 129574-46-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(NMR of carbon-13 and hydrogen in)
- RN 129574-45-4 HCAPLUS
- CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-methyl-9-(phenylmethyl)-, (3 α ,4 α ,9 α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

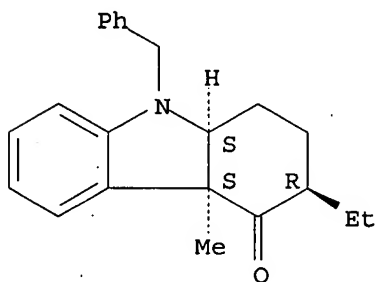


10558931.trn

RN 129574-46-5 HCAPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-methyl-9-(phenylmethyl)-, (3 α ,4 α β ,9 α β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 129574-41-0P 129574-42-1P 129574-43-2P

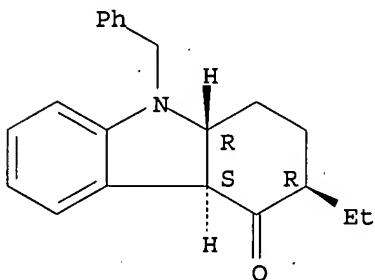
129574-44-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR of)

RN 129574-41-0 HCAPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3 α ,4 α β ,9 α α)- (9CI) (CA INDEX NAME)

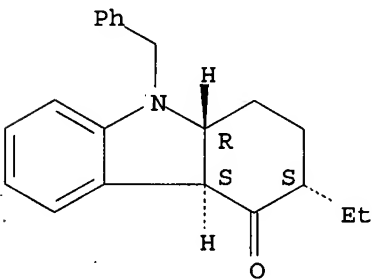
Relative stereochemistry.



RN 129574-42-1 HCAPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3 α ,4 α α ,9 α β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

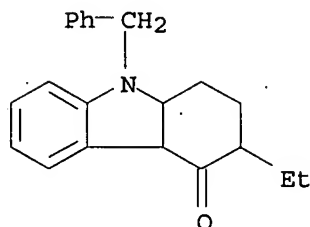


RN 129574-43-2 HCAPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3 α ,4 α α ,9 α α)- (9CI) (CA INDEX NAME)

10558931.trn

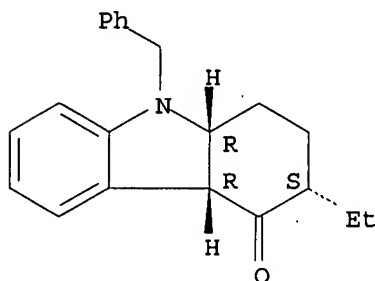
(3 α ,4 α ,9 α) - (9CI) (CA INDEX NAME)



RN 129574-44-3 HCAPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-,
(3 α ,4 α β ,9 α β) - (9CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1987:67041 HCAPLUS

DOCUMENT NUMBER: 106:67041

TITLE: Tetrahydrocarbazoles. Part II. Tricyclic inhibitors
of gastric acid secretion

AUTHOR(S): Canas-Rodriguez, A.; Mateo Bernardo, A.

CORPORATE SOURCE: Chelsea Coll., Univ. London, London, SW3 6LX, UK

SOURCE: Anales de Quimica, Serie C: Quimica Organica y
Bioquimica (1985), 81(3), 254-7

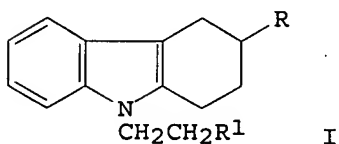
CODEN: AQSBD6; ISSN: 0211-1357

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 106:67041

GI



AB Tetrahydrocarbazoles I (R = Me, Et, CHMe2, CMe3, CH2CMe3; R1 = NMe2, NEt2, 1-pyrrolidinyl, 1-piperidyl) were prepared. Some of them showed gastric secretion inhibitory properties. Structure activity relationships of I were studied.

10558931.trn

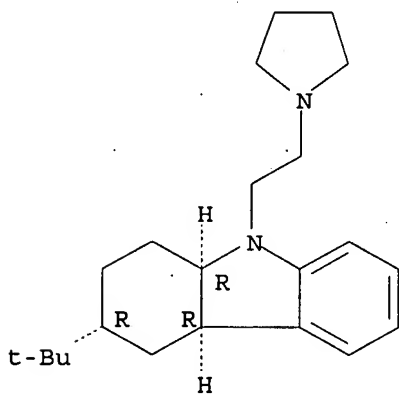
IT 106583-49-7P 106583-67-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and gastric secretion inhibition of)

RN 106583-49-7 HCAPLUS

CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro-9-[2-(1-pyrrolidinyl)ethyl]-, monohydrochloride, (3 α ,4 α ,9 α)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

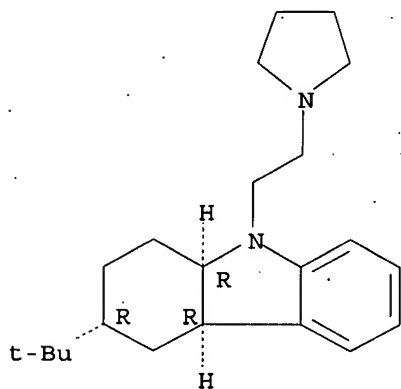


● HCl

RN 106583-67-9 HCAPLUS

CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro-9-[2-(1-pyrrolidinyl)ethyl]-, (3 α ,4 α ,9 α)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1979:22056 HCAPLUS

DOCUMENT NUMBER: 90:22056

TITLE: Substituent effects in saturated systems. An assessment of the transmission of substituent effects by the field, σ -inductive, and π -inductive

10558931.trn

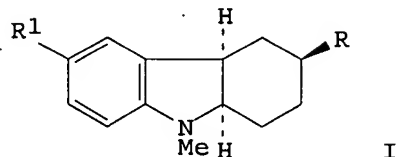
AUTHOR(S):
CORPORATE SOURCE:
SOURCE:

effects in 3- and 6-substituted hexahydrocarbazoles
Utley, James H. P.; Yeboah, Samuel O.
Dep. Chem., Queen Mary Coll., London, UK
Journal of the Chemical Society, Perkin Transactions
2: Physical Organic Chemistry (1972-1999) (1978),
(8), 766-70

CODEN: JCPKBH; ISSN: 0300-9580

DOCUMENT TYPE:
LANGUAGE:
GI

Journal
English



AB The basicities of the hexahydrocarbazoles I (R = H, Me, CH₂OH, CH₂OMe, CH₂CN, R₁ = H; R = H, R₁ = Me, CMe₂CN, CH₂OH, CH₂OMe, CH₂CN) were measured. For substituents of the type CH₂R₂ polar effects are analyzed in terms of the direct field effect operating from the 3-position (R) and the field and π -inductive effect operating in concert across the aromatic portion of the mol. (from R₁). Empirical correlations and the results of calcns. of ΔpK_a using the Kirkwood-Westheimer method show that the field effect is substantial but that relay by the π -inductive effect is greater by a factor of .apprx.2.5.

IT 68384-50-9

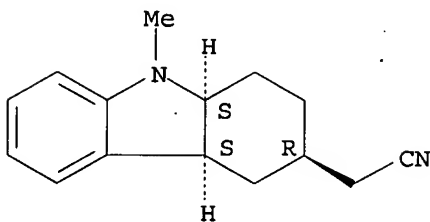
RL: PRP (Properties)

(basicity of, transmission of substituent effect in relation to)

RN 68384-50-9 HCAPLUS

CN 1H-Carbazole-3-acetonitrile, 2,3,4,4a,9,9a-hexahydro-9-methyl-,
(3 α ,4 α β ,9 α β) - (9CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

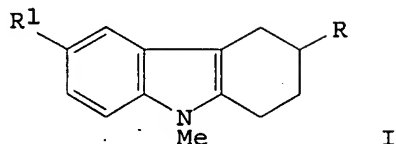
ACCESSION NUMBER: 1978:615158 HCAPLUS

DOCUMENT NUMBER: 89:215158

TITLE: Preparation of a series of 3- and 6-substituted
1,2,3,4-tetra- and 1,2,3,4,4a,9a-hexa-hydrocarbazoles
AUTHOR(S): Utley, James H. P.; Yeboah, Samuel O.
CORPORATE SOURCE: Dep. Chem., Queen Mary Coll., London, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions
1: Organic and Bio-Organic Chemistry (1972-1999)
(1978), (8), 888-92

DOCUMENT TYPE:
LANGUAGE:
GI

CODEN: JCPRB4; ISSN: 0300-922X
Journal
English



AB 4-Ethoxycarbonylcyclohexanone reacted with PhNMeNH₂ in AcOH:HCl under reflux to give 30% tetrahydrocarbazole I (R = CO₂H, R₁ = H), which on reductive methylation (NaH-MeI-DMF) gave 60% I (R = CH₂OMe, R₁ = H) and on p-tolylsulfonylation gave 75% I (R = CH₂O₃SC₆H₄Me-4, R₁ = H) (II). Treatment of II with NaCN-DMF gave 80% I (R = CH₂CN, R₁ = H) and II with pyridine.HCl-DMF gave 70% I (R = CH₂Cl). Bischler reaction of 2-chlorocyclohexanone (III) with 4-H₂NC₆H₄CO₂Et followed by methylation gave 80% I (R = H, R₁ = CO₂Et), which on LiAlH₄ reduction gave 70% I (R = H, R₁ = CH₂OH) (IV). Methylation of IV gave 50% I (R = H, R₁ = CH₂OMe). Bischler reaction of III with 4-H₂NC₆H₄CH₂CN gave 10% 6-cyanomethyl-1,2,3,4-tetrahydrocarbazole which on treatment with MeI gave 70% I (R = H, R₁ = CMe₂CN). Similarly, III with 4-MeNHC₆H₄CH₂CN gave 20% I (R = H, R₁ = CH₂CN). Hydrogenation of I (R = CH₂OH, CH₂OMe, CH₂CN, R₁ = H; R = H, R₁ = CO₂Et, CH₂OH, CH₂OMe, CH₂CN, CMe₂CN) gave the corresponding syn,cis and cis-hexahydrocarbazoles, resp.

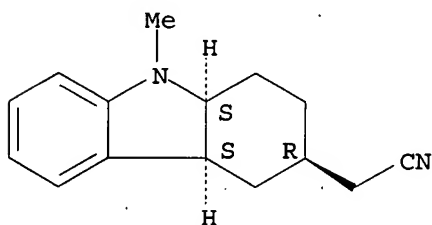
IT 68384-50-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 68384-50-9 HCAPLUS

CN 1H-Carbazole-3-acetonitrile, 2,3,4,4a,9,9a-hexahydro-9-methyl-,
(3 α ,4 α ,9 α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1971:448056 HCAPLUS

DOCUMENT NUMBER: 75:48056

TITLE: Substituent effects in saturated systems. Basicity, reactivity, and stereochemistry in 3- and 6-substituted cis-hexahydrocarbazoles

AUTHOR(S): Utley, J. H. P.; Smith, Alan

CORPORATE SOURCE: Queen Mary Coll., Univ. London, London, UK

SOURCE: Journal of the Chemical Society [Section] B: Physical Organic (1971), (6), 1201-7
CODEN: JCSPAC; ISSN: 0045-6470

DOCUMENT TYPE: Journal
 LANGUAGE: English

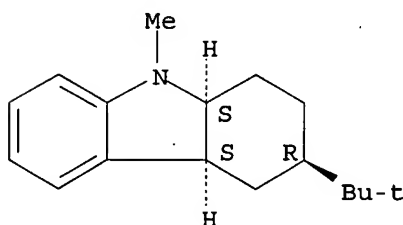
AB Rates of quaternization in MeCN and MeOH and pKa in H₂O and aqueous BuO(CH₂)₂OH were determined for N-methyl-cis-1,2,3,4,4a,9a-hexahydrocarbazoles substituted (Me₃C, Me, MeO) at the 3 and 6 positions. The decrease in basicity caused by 6-Me₃C, syn-3-Me and syn-3-Me₃C substitution is due to steric inhibition of general solvation of the conjugate acid, but this effect is offset by inhibition of H bonding to free base in the 3,3-di-Me derivative. The differences in rates of quaternization accompanying a change of solvent are due to steric effects on H bonding involving the N lone pair and MeOH.

IT 25374-49-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (quaternization of, kinetics of)

RN 25374-49-6 HCAPLUS

CN Carbazole, 3 β -tert-butyl-1,2,3,4,4a,9a-hexahydro-9-methyl- (8CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1970:465901 HCAPLUS

DOCUMENT NUMBER: 73:65901

TITLE: Conformation of syn- and anti-3-substituted cis-hexahydrocarbazoles from nuclear magnetic resonance coupling constants.

AUTHOR(S): Shaw, Derek; Smith, Alan; Utley, J. H. P.

CORPORATE SOURCE: Dep. Chem., Queen Mary Coll., London, UK

SOURCE: Journal of the Chemical Society [Section] B: Physical Organic (1970), (6), 1161-5
 CODEN: JCSPAC; ISSN: 0045-6470

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Double-irradiation expts. were used to interpret the NMR spectra of the methiodides of syn- and anti-3-substituted N-methyl-cis-hexahydrocarbazoles. The Karplus relation and conformational theory were used qual. to rationalize the characteristic splitting patterns and coupling const. involving the ring junction protons, thus distinguishing between alternative conformations. For the syn series and the 3,3-dimethyl compound the alicyclic ring adopts a rigid shallow boat conformation. The anti compds. are probably conformationally mobile at probe temperature

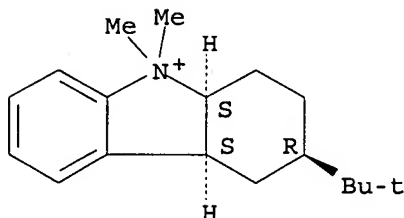
IT 25374-59-8
 RL: PRP (Properties)
 (conformation of)

RN 25374-59-8 HCAPLUS

CN Carbazolium, 3 β -tert-butyl-1,2,3,4,4a,9a-hexahydro-9,9-dimethyl-, iodide (8CI) (CA INDEX NAME)

10558931.trn

Relative stereochemistry.



● I⁻

L25 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1970:55144 HCAPLUS

DOCUMENT NUMBER: 72:55144

TITLE: Configurational isomers of 3-substituted cis-hexahydrocarbazoles

AUTHOR(S): Smith, Alan; Utley, J. H. P.

CORPORATE SOURCE: Dep. Chem., Queen Mary Coll., London, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic (1970), (1), 1-5

CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The preparation and properties of cis-hexahydrocarbazoles (I) substituted (tert-Bu, Me, and MeO) at the 3- and 6-positions are described. The role of protonation in the smooth catalytic hydrogenation of tetrahydrocarbazoles in ethanol-aqueous fluoroboric acid was confirmed. Configurational isomers, defined as syn and anti, were identified in the 3-substituted series of I; their configurations were assigned according to conformational theory and NMR spectroscopic data.

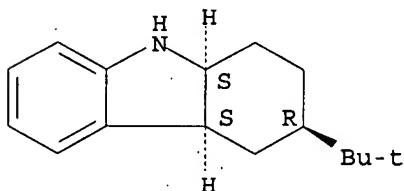
IT 25374-46-3P 25374-49-6P 25374-59-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 25374-46-3 HCAPLUS

CN Carbazole, 3β-tert-butyl-1,2,3,4,4α,9α-hexahydro- (8CI) (CA INDEX NAME)

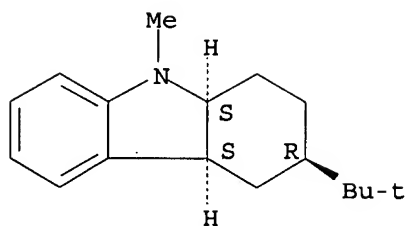
Relative stereochemistry.



RN 25374-49-6 HCAPLUS

CN Carbazole, 3β-tert-butyl-1,2,3,4,4α,9α-hexahydro-9-methyl- (8CI) (CA INDEX NAME)

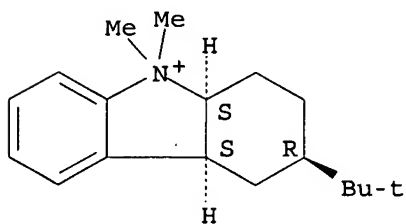
Relative stereochemistry.



RN 25374-59-8 HCAPLUS

CN Carbazolium, 3β-tert-butyl-1,2,3,4,4α,9α-hexahydro-9,9-dimethyl-, iodide (8CI) (CA INDEX NAME)

Relative stereochemistry.

● I⁻

L25 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:35729 HCAPLUS

DOCUMENT NUMBER: 64:35729

ORIGINAL REFERENCE NO.: 64:6602a-b

TITLE: Some studies of the formation and structure of melanins

AUTHOR(S): Swan, George Albert

CORPORATE SOURCE: Univ. Newcastle-upon-Tyne, UK

SOURCE: Rend. Accad. Sci. Fis. Mat. (Soc. Nazl. Sci., Napoli) (1964), 31, 212-31

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In addition to a literature review on the subject (25 references), studies are described of the formation of melanins (I), (a) enzymically, and (b) by autoxidn. from 2,3-(HO)2C6H3CH2CH(CO2H)NH2 (II) and 2,3-(HO)2C6H3CH2CH2NH2 (III). When II and III were labeled with D in the α or β position of the side chain and then converted to I, large retention of D was observed in the I. This suggests that the I are not polymers composed entirely of indole-5,6-quinone, but that they also contain uncyclized units of the precursors (or quinones derived from these) or (more probably) units of 2,3-dihydroindole-5,6-quinone. When I prepared from II-carboxy-14C was oxidized, the resulting pyrrole-2,3,5-tricarboxylic acid was radioactive while the pyrrole-2,3-dicarboxylic acid was inactive.

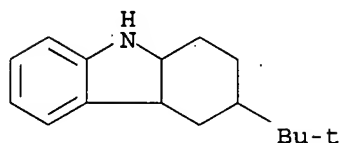
IT 6731-89-1

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 6731-89-1 HCAPLUS

CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro- (9CI). (CA

INDEX NAME)



L25 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:35728 HCAPLUS

DOCUMENT NUMBER: 64:35728

ORIGINAL REFERENCE NO.: 64:6601g-h,6602a

TITLE: Catalytic hydrogenation of indoles

AUTHOR(S): Smith, A.; Utley, J. H. P.

CORPORATE SOURCE: Queen Mary Coll., London

SOURCE: Chemical Communications (London) (1965), (18), 427-8

CODEN: CCOMA8; ISSN: 0009-241X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 64:35728

GI For diagram(s), see printed CA Issue.

AB Indoles (I), 1 g., were hydrogenated in EtOH \cdot HBF₄ solution over 0.01-0.5 g. PtO₂ at 1 atmospheric and room temperature to give quant. the corresponding indolines

(R1, R2, and m.p. or b.p./mm. given): H, H, m. 95-6°; Me, H, m. 30-1°, H, Me, m. 54-6°; tert-Bu, H, m. 64-5°; H, tert-Bu, m. 75-7°.

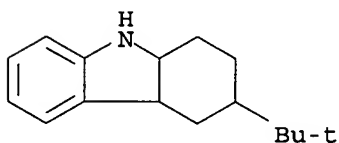
IT 6731-89-1P, Carbazole, 3-tert-butyl-1,2,3,4,4a,9a-hexahydro-

RL: PREP (Preparation)

(formation in 3-tert-butyl-1,2,3,4-tetrahydrocarbazole hydrogenation)

RN 6731-89-1 HCAPLUS

CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)



L25 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1952:57425 HCAPLUS

DOCUMENT NUMBER: 46:57425

ORIGINAL REFERENCE NO.: 46:9616h-i,9617a-e

TITLE: Imidazolines

INVENTOR(S): Hartman, Max; Studer, Siegfried

PATENT ASSIGNEE(S): C I B A Pharmaceutical Products, Inc.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

KIND

DATE

APPLICATION NO.

DATE

US 2569415 19510925 US 1948-65067 19481213

AB 2-(9-Carbazolylalkyl)imidazolines (I) and their salts of inorg. or organic acids are prepared by treating a 9-carbazolealkanecarboxylic acid or its reactive acid derivative with a N-unsubstituted alkylenediamine or its reactive N-derivative I and their salts exhibit an action similar to that of adrenaline. 9-Carbazoleacetic acid 45 and (CH₂NH₂)₂.H₂O 16 in warm alc. 300 parts by weight is mixed with 1 equivalent HCl in EtOH, the whole heated to about 230°, the EtOH distilled off, the mixture stirred 0.5 h., 28.4 parts P2O₅ added, the temperature kept 1.5 h. at 230°, and the mass cooled, pulverized, and extracted with hot H₂O; the filtered solution yields 2-(9-carbazolylmethyl)-2-imidazoline, m. 232-234° (from EtOH). (HCl salt, m. 270-2°). Et 1,2,3,4,-tetrahydro-9-carbazoleacetate yields 2-(1,2,3,4-tetrahydro-9-carbazolylmethyl)-2-imidazoline, m. 180-1°; HCl salt, decompose 275-7.5°. 9-(Cyanomethyl)-1,2,8,4-tetrahydrocarbazole yields 2-(1,2,3,4-tetrahydro-9-carbazolylmethyl)-2-imidazoline, m. 132-3°, (HCl salt, m. 210-11° (decomposition)). 9-(2-Cyanoethyl)carbazole produces 2-[2-(9-carbazolyl)ethyl]-2-imidazoline (HCl salt, m. 253°). 2-[2-(1,2,3,4-Tetrahydro-9-carbazolyl)ethyl]-2-imidazoline (HCl salt, m. 213-15°), is prepared from 9-(2-cyanoethyl)tetrahydrocarbazole. 2-Chlorocyclohexanone condensed with anilines substituted in the 4-position yields the 5,6,7,8-tetrahydrocarbazoles (II) substituted in the 3-position; the 3-PhO compound b0.1 209-10°, m. 141-3°. The II by reduction with Sn and concentrated HCl in EtOH yield the corresponding carbazoles: 3-Me, b0.5 114-15°; 3-MeO, b0.4 128-9°; 3-EtO, b0.18 132-4°; 3-PhO, b0.2 196-8°; 3-Cl, b0.38 134°, m. 62-4°. By treating the above carbazoles with trioxymethylene and aqueous KCN solution in glacial AcOH at 5-10° and then stirring 20 h. at room temperature may be prepared the following 9-(cyanomethyl)carbazoles: 3-Me, b0.32 157-8°; 3-MeO, m. 107-8°; 3-EtO, m. 102.5-3.5°; 3-PhO, m. 119.5-20.5°; 3-Cl, m. 81-2°. Upon dehydrogenation with chloranil in boiling xylene, the substituted 9-(cyanomethyl)carbazoles are converted into the corresponding 9-(cyanomethyl)carbazoles. 3-Methoxy-9-(cyanomethyl)carbazole (III), m. 116-17°, 17 refluxed 1 h. at a bath temperature of 220° with p-MeC₆H₄SO₃NH₃CH₂CH₂NH₂ 16.3 parts, the crystalline product dissolved in dilute EtOH, the solution made alkaline to phenolphthalein with 5 N NaOH, the precipitated crystalline powder dissolved in CH₂Cl₂, the solution dried over KOH and the CH₂Cl₂ evaporated gives 91.3% 2-(3-methoxy-9-carbazolylmethyl)-2-imidazoline (IV), m. 182-3° (after distillation in a high vacuum and recrystn. from EtOH); HCl salt, m. 227-8°. Similarly, the following analogs of III yield the corresponding analogs of IV. 3-Me analog of III, 9-(cyanomethyl)carbazole, m. 141-2°; of IV, m. 171-2.5° (HCl salt, m. 271-3°). 3-EtO analog of III, m. 95-7°; of IV, m. 164-5° (HCl salt, m. 242-2.5°). 3-PhO analog of III, m. 105-6°; of IV, m. 172.5-3.5° (HCl salt, m. 271-2°). 3-Cl analog of III; of IV, m. 213-15° (HCl salt, m. 263-5°).

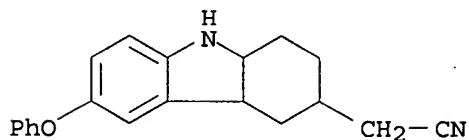
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RL: PREP (Preparation)
(preparation of)

RN 854825-67-5 HCAPLUS

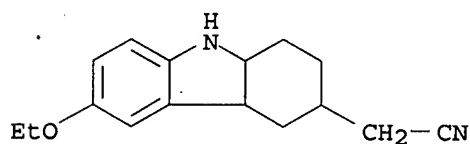
10558931.trn

CN 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-phenoxy- (5CI) (CA
INDEX NAME)



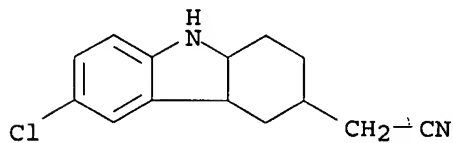
RN 854825-68-6 HCAPLUS

CN 9-Carbazoleacetonitrile, 6-ethoxy-1,2,3,4,4a,9a-hexahydro- (5CI) (CA
INDEX NAME)



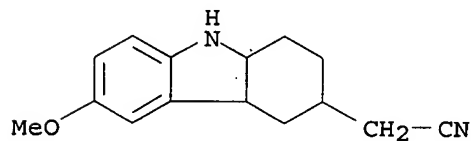
RN 854825-69-7 HCAPLUS

CN 9-Carbazoleacetonitrile, 6-chloro-1,2,3,4,4a,9a-hexahydro- (5CI) (CA
INDEX NAME)



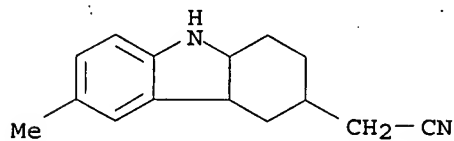
RN 855712-17-3 HCAPLUS

CN 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-methoxy- (5CI) (CA
INDEX NAME)



RN 855712-19-5 HCAPLUS

CN 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-methyl- (5CI) (CA
INDEX NAME)



10558931.trn

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L34 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:790472 HCAPLUS

DOCUMENT NUMBER: 133:335158

TITLE: Preparation of 3,3-substituted indolines as
progesterone receptor antagonists

INVENTOR(S): Ullrich, John W.; Fensome, Andrew; Zhi, Lin; Jones,
Todd K.; Marschke, Keith B.; Tegley, Christopher M.

PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand
Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 45 pp.

CODEN: PIXXD2

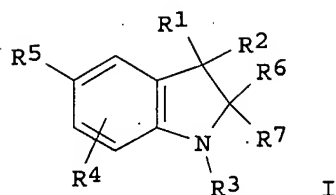
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066554	A1	20001109	WO 2000-US11464	20000501 <--
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6417214	B1	20020709	US 2000-552352	20000419 <--
CA 2371629	A1	20001109	CA 2000-2371629	20000501 <--
EP 1175397	A1	20020130	EP 2000-930201	20000501 <--
EP 1175397	B1	20040818		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
JP 2002543181	T	20021217	JP 2000-615385	20000501 <--
AT 273951	T	20040915	AT 2000-930201	20000501
PT 1175397	T	20050131	PT 2000-930201	20000501
ES 2226838	T3	20050401	ES 2000-930201	20000501
US 2003008909	A1	20030109	US 2002-131379	20020424 <--
US 6835744	B2	20041228		
HK 1043986	A1	20050401	HK 2002-104852	20020628
PRIORITY APPLN. INFO.:			US 1999-183061P	P 19990504
			US 2000-552352	A1 20000419
			WO 2000-US11464	W 20000501
OTHER SOURCE(S):	MARPAT 133:335158			
GI				



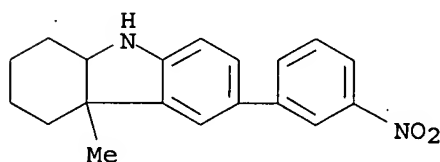
AB The title compds. [I; R1, R2 = H, OH, OAc, etc.; or R1 and R2 are joined to form a ring comprising CH₂(CH₂)_nCH₂, CH₂CH₂CMe₂CH₂CH₂, O(CH₂)_mCH₂, etc.; or R1 and R2 together comprise a double bond to CMe₂, C(cycloalkyl), O, C(cycloether); n = 0-5; m = 1-4; R3 = H, OH, NH₂, etc.; R4 = H, halo, CN, etc.; R5 = optionally substituted Ph, a 5-6 membered heterocycle, a 4- or 7-substituted indole, substituted benzothiophene; R6, R7 = H, Me, Et, etc.] which are progesterone receptor antagonists, and are useful in inducing contraception, and treating or preventing benign or malignant neoplastic disease, were prepared Thus reacting 5-bromo-2,3,3-trimethyl-2,3-dihydro-1H-indole (preparation given) with 3-nitrophenylboronic acid in the presence of Pd(PPh₃)₄ afforded 82% I [R1, R2 = Me; R3, R4 = H; R5 = 3-O₂NC₆H₄; R6 = Me; R7 = H]. In general, compds. I were effective at 0.5-500 mg/kg/day.

IT 304468-33-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3,3-substituted indolines as progesterone receptor antagonists)

RN 304468-33-5 HCAPLUS

CN 1H-Carbazole, 2,3,4,4a,9,9a-hexahydro-4a-methyl-6-(3-nitrophenyl)- (9CI)
(CA INDEX NAME)

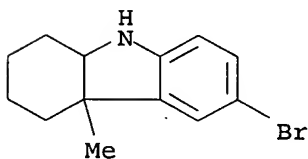


IT 304468-40-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3,3-substituted indolines as progesterone receptor antagonists)

RN 304468-40-4 HCAPLUS

CN 1H-Carbazole, 6-bromo-2,3,4,4a,9,9a-hexahydro-4a-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:790349 HCAPLUS

DOCUMENT NUMBER: 133:350134

TITLE: Preparation of 3,3-substituted indolines useful in contraceptive compositions

INVENTOR(S): Grubb, Gary S.; Zhi, Lin; Jones, Todd K.; Tegley, Christopher M.; Ullrich, John W.; Fensome, Andrew; Wrobel, Jay E.; Edwards, James P.

PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

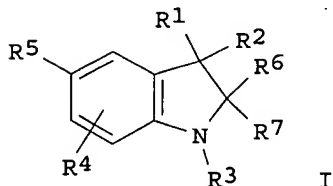
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WO 2000066166	A1	20001109	WO 2000-US11748	20000501 <--
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RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6329416	B1	20011211	US 2000-552631	20000419 <--
CA 2372591	A1	20001109	CA 2000-2372591	20000501 <--
EP 1173211	A1	20020123	EP 2000-928667	20000501 <--
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
JP 2002543157	T	20021217	JP 2000-615050	20000501 <--
US 2002035099	A1	20020321	US 2001-977790	20011015 <--
US 6503939	B2	20030107		

PRIORITY APPLN. INFO.:

US 1999-183057P P 19990504
US 2000-552631 A1 20000419
WO 2000-US11748 W 20000501

OTHER SOURCE(S): MARPAT 133:350134

GI



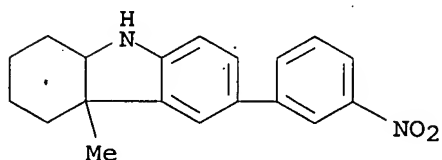
AB The title compds. [I; R1, R2 = H, OH, OAc, etc.; or R1 and R2 are joined to form a ring comprising CH₂(CH₂)_nCH₂, CH₂CH₂CMe₂CH₂CH₂, O(CH₂)_mCH₂, etc.; or R1 and R2 together comprise a double bond to CMe₂, C(cycloalkyl), O, C(cycloether); n = 0-5; m = 1-4; R3 = H, OH, NH₂, etc.; R4 = H, halo, CN, etc.; R5 = optionally substituted Ph, a 5-6 membered heterocycle, a 4- or 7-substituted indole, substituted benzothiophene; R6, R7 = H, Me, Et, etc.] which are progesterone receptor antagonists, and are useful in inducing contraception, and treating or preventing benign or malignant neoplastic disease, were prepared Thus reacting 5-bromo-2,3,3-trimethyl-2,3-dihydro-1H-indole (preparation given) with 3-nitrophenylboronic acid in the presence of Pd(PPh₃)₄ afforded 82% I [R1, R2 = Me; R3, R4 = H; R5 = 3-O₂NC₆H₄; R6 = Me; R7 = H]. In general, compds. I were effective at 0.5-500 mg/kg/day..

IT 304468-33-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3,3-substituted indolines as progesterone receptor antagonists)

RN 304468-33-5 HCAPLUS

CN 1H-Carbazole, 2,3,4,4a,9,9a-hexahydro-4a-methyl-6-(3-nitrophenyl)- (9CI)
(CA INDEX NAME)

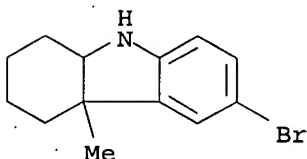


IT 304468-40-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3,3-substituted indolines as progesterone receptor antagonists)

RN 304468-40-4 HCAPLUS

CN 1H-Carbazole, 6-bromo-2,3,4,4a,9,9a-hexahydro-4a-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:787188 HCAPLUS

DOCUMENT NUMBER: 123:198832

TITLE: Tetracyclic condensed heterocyclic compounds for the treatment of senile dementia.

INVENTOR(S): Goto, Giichi; Ishihara, Yuji; Miyamoto, Masaomi

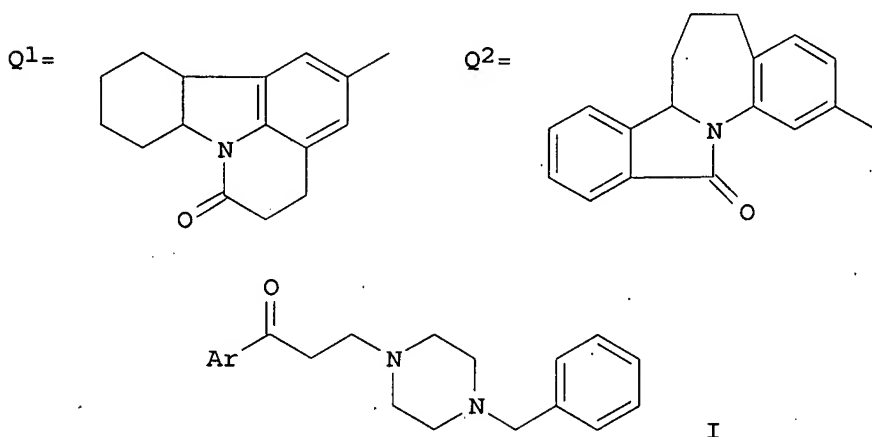
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

10558931.trn

SOURCE: Eur. Pat. Appl., 53 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 655451	A1	19950531	EP 1994-118734	19941129 <--
EP 655451	B1	20010620		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
US 5620973	A	19970415	US 1994-330133	19941025 <--
CA 2136913	A1	19950531	CA 1994-2136913	19941129 <--
JP 07309835	A	19951128	JP 1994-294754	19941129 <--
AT 202354	T	20010715	AT 1994-118734	19941129 <--
US 5814642	A	19980929	US 1996-681911	19960730 <--
PRIORITY APPLN. INFO.:			JP 1993-299799	A 19931130
			JP 1994-55984	A 19940325
			US 1994-330133	A3 19941025

OTHER SOURCE(S): CASREACT 123:198832; MARPAT 123:198832
 GI



AB Title compds. ArCO(CHR1)nY [Ar = (un)substituted tetracyclic fused heterocyclic group; R1 = H or (un)substituted hydrocarbyl; n = 1-10; Y = amino or N-containing saturated (un)substituted heterocyclic group] and their salts are claimed. The compds. show excellent cholinesterase inhibitory activity and monoamine uptake inhibitory activity, thus being useful as therapeutic and/or prophylactic medicaments for senile dementia and Alzheimer's disease, and also as antidepressants. For example, 1,2,3,4,4a,9a-hexahydrocarbazole underwent N-acylation by ClCH2CH2COCl, Friedel-Crafts cyclization by AlCl3, and Friedel-Crafts acylation by treatment with both ClCH2CH2COCl and AlCl3, to give pyridocarbazolone derivative ArCOCH2CH2Cl [Ar = Q1]. Reaction of the latter with 1-benzylpiperazine gave title compound I [Ar = Q1] as the di-HCl salt. The similarly prepared compound I [Ar = Q2] had IC50 of 0.0164 µM for inhibition of rat cerebral cholinesterase in vitro, vs. 0.220 for physostigmine and 0.300 for THA. The same compound was also as potent as imipramine in a monoamine uptake inhibitor assay.

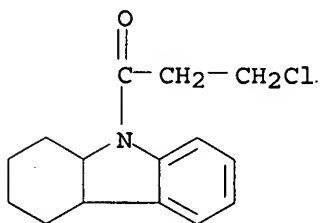
IT 167633-68-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(intermediate; preparation of tetracyclic heterocyclics for treatment of senile dementia)

RN 167633-68-3 HCAPLUS

CN 1H-Carbazole, 9-(3-chloro-1-oxopropyl)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)



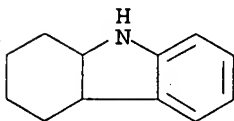
IT 1775-86-6, 1,2,3,4,4a,9a-Hexahydrocarbazole

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of tetracyclic heterocyclics for treatment of senile dementia)

RN 1775-86-6 HCAPLUS

CN 1H-Carbazole, 2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)



L34 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1981:47136 HCAPLUS

DOCUMENT NUMBER: 94:47136

TITLE: Tetrahydrocarbazoles and pharmaceutical compositions for treating heart failure in mammals

INVENTOR(S): Mooradian, Aram

PATENT ASSIGNEE(S): Sterling Drug Inc., USA

SOURCE: U.S., 7 pp. Cont.-in-part of U.S. Ser. No. 465,238, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

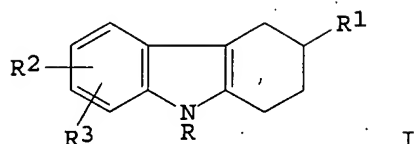
FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4224335	A	19800923	US 1976-651882	19760123 <--
US 3642816	A	19720215	US 1967-659606	19670810 <--
US 3959309	A	19760525	US 1973-425205	19731217 <--
PRIORITY APPLN. INFO.:			US 1967-659606	A2 19670810
			US 1969-793545	A2 19690123
			US 1971-172206	A2 19710816
			US 1973-425205	A2 19731217
			US 1974-465238	A2 19740429
			CA 1968-10686	A 19680124

OTHER SOURCE(S):
GI

MARPAT 94:47136



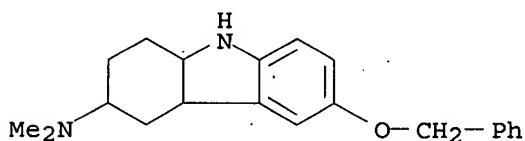
AB The carbazoles I (R = H, Me; R1 = NH₂, EtNH, Me₂N; R2 = 5-, 6-, 7-HO; R3 = H, 7-F, 7-HO) were prepared. Thus, m-PhCH₂OC₆H₄NMeNH₂.HCl was cyclized with 4-(dimethylamino)cyclohexanone to give I (R = Me, R1 = Me₂N, R2 = 7-PhCH₂O, R3 = H), which was debenzylated to give I (R = Me, R1 = Me₂N, R2 = 7-HO, R3 = H). I underwent cardiotoxic tests and were found useful for treatment of congestive heart failure in mammals.

IT 76243-30-6 76243-31-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(debenzylation of)

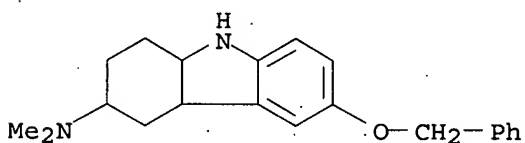
RN 76243-30-6 HCAPLUS

CN 1H-Carbazol-3-amine, 2,3,4,4a,9,9a-hexahydro-N,N-dimethyl-6-(phenylmethoxy)- (9CI) (CA INDEX NAME)



RN 76243-31-7 HCAPLUS

CN 1H-Carbazol-3-amine, 2,3,4,4a,9,9a-hexahydro-N,N-dimethyl-6-(phenylmethoxy)-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

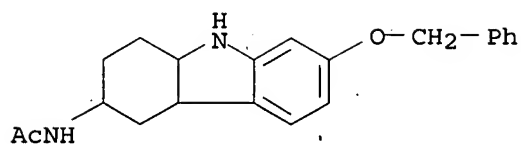
IT 76243-19-1P 76243-22-6P 76243-27-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and debenzylation of)

RN 76243-19-1 HCAPLUS

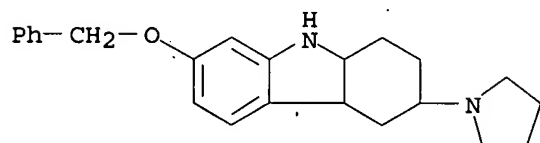
CN Acetamide, N-[2,3,4,4a,9,9a-hexahydro-7-(phenylmethoxy)-1H-carbazol-3-yl]- (9CI) (CA INDEX NAME)

10558931.trn



RN 76243-22-6 HCAPLUS

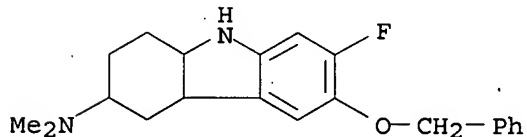
CN 1H-Carbazole, 2,3,4,4a,9,9a-hexahydro-7-(phenylmethoxy)-3-(1-pyrrolidinyl)-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

RN 76243-27-1 HCAPLUS

CN 1H-Carbazol-3-amine, 7-fluoro-2,3,4,4a,9,9a-hexahydro-N,N-dimethyl-6-(phenylmethoxy)-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

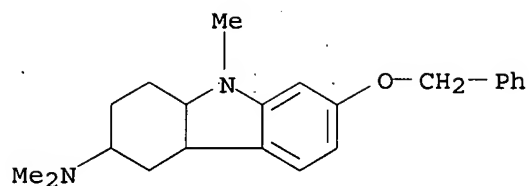
IT 76243-05-5P 76243-06-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrogenolysis of)

RN 76243-05-5 HCAPLUS

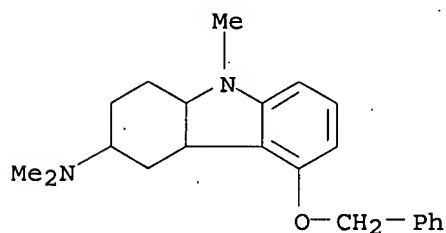
CN 1H-Carbazol-3-amine, 2,3,4,4a,9,9a-hexahydro-N,N,9-trimethyl-7-(phenylmethoxy)-, hydrochloride (9CI) (CA INDEX NAME)

10558931.trn



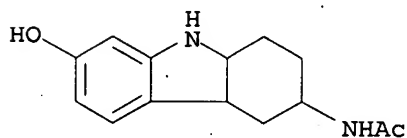
●x HCl

RN 76243-06-6 HCAPLUS
CN 1H-Carbazol-3-amine, 2,3,4,4a,9,9a-hexahydro-N,N,9-trimethyl-5-(phenylmethoxy)-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

IT 76243-20-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrolysis of)
RN 76243-20-4 HCAPLUS
CN Acetamide, N-(2,3,4,4a,9,9a-hexahydro-7-hydroxy-1H-carbazol-3-yl)- (9CI) (CA INDEX NAME)

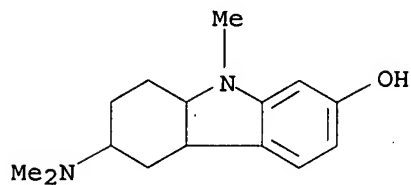


IT 76243-10-2P 76243-14-6P 76243-32-8P
76254-53-0P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
RN 76243-10-2 HCAPLUS
CN 1H-Carbazol-7-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-9-methyl-, methanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

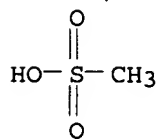
10558931.trn

CRN 76243-09-9
CMF C15 H22 N2 O

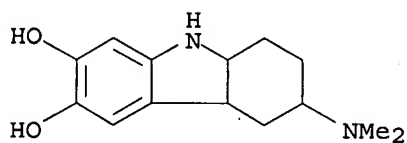


CM 2

CRN 75-75-2
CMF C H4 O3 S



RN 76243-14-6 HCAPLUS
CN 1H-Carbazole-6,7-diol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-,
hydrobromide (9CI) (CA INDEX NAME)

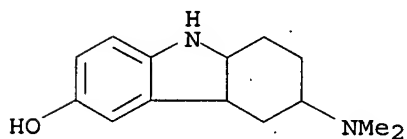


● x HBr

RN 76243-32-8 HCAPLUS
CN 1H-Carbazol-6-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-,
monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 76243-03-3
CMF C14 H20 N2 O

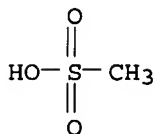


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CM 2

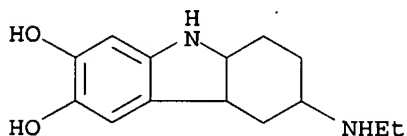
CRN 75-75-2

CMF C H4 O3 S



RN 76254-53-0 HCAPLUS

CN 1H-Carbazole-6,7-diol, 3-(ethylamino)-2,3,4,4a,9,9a-hexahydro-, hydrobromide (9CI) (CA INDEX NAME)



● x HBr

IT 76243-03-3P 76243-04-4P 76243-07-7P

76243-08-8P 76243-13-5P 76243-17-9P

76243-18-0P 76243-21-5P 76243-23-7P

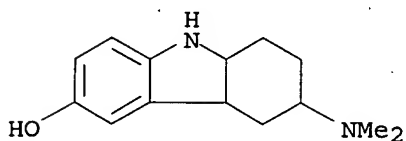
76243-29-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, for treatment of congestive heart failure)

RN 76243-03-3 HCAPLUS

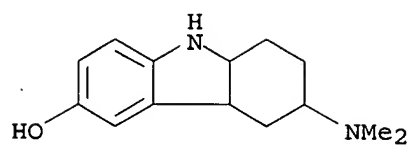
CN 1H-Carbazol-6-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)



RN 76243-04-4 HCAPLUS

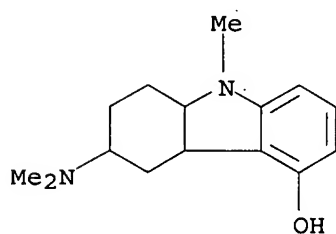
CN 1H-Carbazol-6-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-, hydrochloride (9CI) (CA INDEX NAME)

10558931.trn



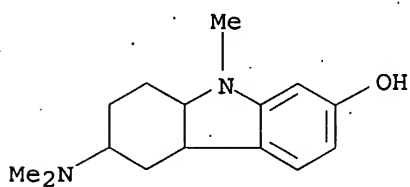
●x HCl

RN 76243-07-7 HCAPLUS
CN 1H-Carbazol-5-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-9-methyl-,
hydrochloride (9CI) (CA INDEX NAME)



●x HCl

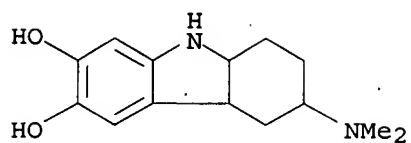
RN 76243-08-8 HCAPLUS
CN 1H-Carbazol-7-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-9-methyl-,
hydrochloride (9CI) (CA INDEX NAME)



●x HCl

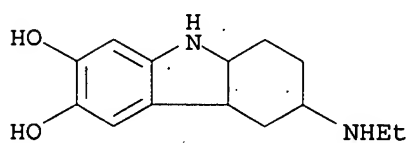
RN 76243-13-5 HCAPLUS
CN 1H-Carbazole-6,7-diol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-,
hydrochloride (9CI) (CA INDEX NAME)

10558931.trn



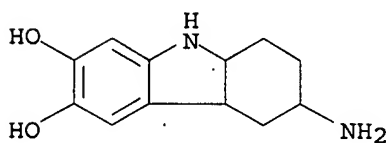
●x HCl

RN 76243-17-9 HCAPLUS
CN 1H-Carbazole-6,7-diol, 3-(ethylamino)-2,3,4,4a,9,9a-hexahydro-,
hydrochloride (9CI) (CA INDEX NAME)



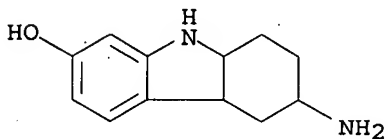
●x HCl

RN 76243-18-0 HCAPLUS
CN 1H-Carbazole-6,7-diol, 3-amino-2,3,4,4a,9,9a-hexahydro-, hydrochloride
(9CI) (CA INDEX NAME)



●x HCl

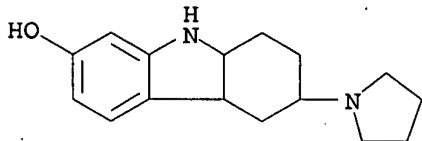
RN 76243-21-5 HCAPLUS
CN 1H-Carbazol-7-ol, 3-amino-2,3,4,4a,9,9a-hexahydro-, hydrochloride (9CI)
(CA INDEX NAME)



●x HCl

10558931.trn

RN 76243-23-7 HCAPLUS
CN 1H-Carbazol-7-ol, 2,3,4,4a,9,9a-hexahydro-3-(1-pyrrolidinyl)-,
hydrochloride (9CI) (CA INDEX NAME)

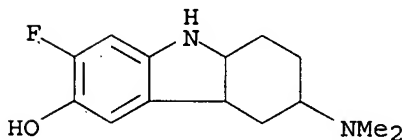


● x HCl

RN 76243-29-3 HCAPLUS
CN 1H-Carbazol-6-ol, 3-(dimethylamino)-7-fluoro-2,3,4,4a,9,9a-hexahydro-,
monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

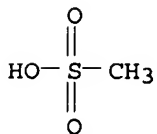
CM 1

CRN 76243-28-2
CMF C14 H19 F N2 O



CM 2

CRN 75-75-2
CMF C H4 O3 S



=> log y

COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
120.93	1505.14
SINCE FILE	TOTAL
ENTRY	SESSION
-14.82	-14.82

STN INTERNATIONAL LOGOFF AT 14:37:48 ON 10 AUG 2007

08/10/2007

Page 58